Part 1. Energies and Cartesian coordinates

Singlet V_4O_{10} (1)

Gasphase Energy: -1038.12627279660 hartrees

Zero Point Energy: 24.675 kcal/mol

Coordinates:

O1	3.4396030928	0.0007324194	0.0000000000
V2	1.8671732077	0.0001123599	0.0000000000
O3	1.1635214411	1.6453188164	0.0000000000
O4	1.1637221815	-0.8229427712	1.4248689206
O5	1.1637221815	-0.8229427712	-1.4248689206
V6	-0.6221116976	-0.8801371208	1.5245388677
V7	-0.6221116976	-0.8801371208	-1.5245388677
V8	-0.6223723882	1.7602297709	0.0000000000
O9	-1.1643593043	0.8224172862	-1.4244457758
O10	-1.1643001918	-1.6444704227	0.0000000000
O11	-1.1465683202	-1.6217925876	-2.8082052772
O12	-1.1643593043	0.8224172862	1.4244457758
O13	-1.1465683202	-1.6217925876	2.8082052772
O14	-1.1462525582	3.2428391043	0.0000000000

Methane

Gasphase Energy: -40.52321631160 hartrees

Zero Point Energy: 28.242 kcal/mol

Coordinates:

C1	-0.0000064895	0.0000213426	0.0000000000
H2	1.0922369424	0.0001073415	0.0000000000
H3	-0.3643527444	1.0296589841	0.0000000000
H4	-0.3639034640	-0.5150102240	0.8917807258
H5	-0.3639034640	-0.5150102240	-0.8917807258

TsA

Gasphase Energy: -1078.51347520169 hartrees

Zero Point Energy: 52.217 kcal/mol

Coordinates:

O1	-1.2588034981	-2.3762458315	-.0924398619
V2	-1.2680237679	-.7980925482	-.1073863990
O3	.3614729568	-.1097350959	-.1393097013
O4	-2.1400763346	-.0446038229	1.2714081019
O5	-2.0368252666	-.1143017865	-1.5689275057
V6	-2.3722958955	1.7316176027	1.4017192007
V7	-2.1219892185	1.6732857785	-1.5977266185
V8	.4585630008	1.6694381339	.3018654244
O9	-.4671972729	2.1544854062	-1.1944237192
O10	-3.0570120448	2.2238068813	-.1736180457
O11	-2.6307964477	2.2683763833	-2.9672770670
O12	-.7658157573	2.4762463515	1.4023451371
O13	-3.2529357062	2.1875898980	2.6294533451
O14	1.9823707073	2.2679983483	.4150743973
H15	.5965394879	.8855121057	1.7095269536
C16	2.2988352683	1.3617893651	2.1586495737
H17	2.3824224065	.2806485579	2.1065708243
H18	3.2245349588	1.8826910337	1.9465321286
H19	1.7392993647	1.7813460974	2.9888516477

ProA

Gasphase Energy: -1078.57929770795 hartrees

Zero Point Energy: 53.538 kcal/mol

Coordinates:

O1	-1.3792897284	-2.8201430613	.2339477525
V2	-1.5309572570	-1.2498210497	.2067505916
O3	.0107371016	-.4147783136	.3366613502
O4	-2.6199063695	-.5422056412	1.4710198365
O5	-2.1881775461	-.6601384881	-1.3444785128
V6	-2.9443511299	1.2047225579	1.5268156451
V7	-2.3390283471	1.1211005409	-1.4353219855
V8	-.0020630199	1.3717650950	.8116573037
O9	-.7901010499	1.6765401655	-.8791681058
O10	-3.4579043543	1.6488749087	-.0947772217
O11	-2.7170398777	1.6667737855	-2.8679405257
O12	-1.3441236274	2.0821303431	1.6801968498
O13	-4.0010186758	1.6180174922	2.6206999881
O14	1.5047434863	2.1458928691	1.0293038997
C15	2.8832049564	1.9745114852	.6935972839
H16	.1018663251	.5158598819	2.1326408582
H17	3.0526108073	.9809014886	.2698074212
H18	3.1508287296	2.7480599353	-.0307667959
H19	3.4654530502	2.0993026565	1.6099280327

TsB

Gasphase Energy: -1078.56728545624 hartrees

Zero Point Energy: 51.364 kcal/mol

Coordinates:

O1	-.6054219561	2.8362240324	-2.0470073980
V2	-.6334180598	1.5484550775	-1.1404093228
O3	.6627319176	1.5280665706	.0948873749
O4	-.5534570812	.0139077390	-2.0533521143
O5	-2.1067816273	1.4404836368	-.1433727326
V6	-.6260551686	-1.5474013169	-1.1583069870
V7	-2.2325597902	-.0217159373	.8861181646
V8	.9619453525	.0048397541	.9759821622
O9	-.6689330961	-.0283436951	1.7406780848
O10	-2.1171822702	-1.4534877241	-.1705543658
O11	-3.4842734806	-.0306639842	1.8426765069
O12	.6441206265	-1.5342461603	.0723807244
O13	-.5786279363	-2.8303812927	-2.0714693283
O14	2.2450472716	.0268106416	2.0547077997
C15	2.8947214107	-.0883202985	-.4702463338
H16	3.3078167190	-1.0977882334	-.4812062369
H17	2.2892610657	.0971475459	-1.3522661701
H18	3.6471635772	.7008078561	-.3719657902
H19	2.8248461517	-.0012582081	1.0900595828

ProB

Gasphase Energy: -1078.60833152840 hartrees

Zero Point Energy: 53.795 kcal/mol

Coordinates:

O1	-1.1726658454	-3.0363063078	-.1018836690
V2	-1.1551192729	-1.4611261502	-.0898060182
O3	.5341469231	-.7443064560	-.0640031848
O4	-1.9121686170	-.8100009070	1.3450551828
O5	-2.0207737843	-.7417504827	-1.4687643381
V6	-1.9596082786	1.0257036109	1.4046059879
V7	-2.1632509547	1.0526683112	-1.5806475319
V8	.7370920897	.9190678831	-.5058189368
O9	-.5118829763	1.7255321044	-1.5147406633
O10	-2.8950193724	1.5588841442	-.0589620695
O11	-2.9810284512	1.5549103462	-2.8318216993
O12	-.3614742277	1.4881289993	1.0452968579
O13	-2.4702630032	1.6381498265	2.7695704948
O14	1.9294287022	.8052764153	-1.7839485948
C15	2.1251289070	1.9970630887	.5474923869
H16	2.2707445772	1.4779837254	-2.3910858239
H17	2.0224413469	2.9995126360	.1181627167
H18	1.8393049519	1.9805531679	1.5956020570
H19	3.0996876420	1.5570806082	.3403748126

TsC

Gasphase Energy: -1078.57931498618 hartrees

Zero Point Energy: 48.256 kcal/mol

Coordinates:

V1	1.2590029027	-1.9324498300	2.7201356841
O2	1.2892804795	-0.1329413037	2.7059275975
O3	-0.4773371325	-2.3712677614	2.7509762372
O4	1.8546613804	-2.3801745539	1.0734914378
V5	-1.5055248616	-1.6662687204	1.4664052535
V6	1.0090275841	-1.7372356596	-0.3419370865
V7	0.3771941479	0.7708337806	1.4832336420
O8	1.0923266325	0.1533613916	-0.1700215082
O9	-0.6980783664	-2.1228604496	-0.0813940595
O10	1.5760867357	-2.2607487591	-1.7180704061
O11	-1.2705053619	0.1182941423	1.5639259804
O12	-3.0191850136	-2.1025523828	1.5145126393
O13	0.4609231455	2.3358250881	1.6609568377
O14	2.1217132300	-2.5433939297	3.8893056732
C15	2.1315010044	1.6653032680	-1.9634341123
H16	2.2839922443	0.9631901655	-2.7816609195
H17	1.3572811282	2.4138873109	-2.1226157130
H18	3.0366540612	2.0232296767	-1.4758831849
H19	1.5768328719	0.8676636631	-1.0061958792

ProC

Gasphase Energy: -1078.59148107999 hartrees

Zero Point Energy: 49.824 kcal/mol

Coordinates:

O1	-0.6161708852	-3.8126088072	0.4478480372
V2	-0.6884089510	-2.2439870261	0.5916987471
O3	0.9391667566	-1.4488048096	0.5439432138
O4	-1.4835684580	-1.6419329786	2.0791273758
O5	-1.5467388432	-1.4423570227	-0.7865300501
V6	-1.5825067058	0.1364127873	2.2681942811
V7	-1.7488130878	0.3106205201	-0.8332382597
V8	1.0932762837	0.3027667184	0.6898832878
O9	0.0655138861	0.9670309913	-0.8008978773
O10	-2.3708974701	0.7520293089	0.7585337412
O11	-2.6662095901	0.8020128930	-2.0199123243
O12	0.1142627057	0.7460882711	2.0890370851
O13	-2.2867749553	0.6417962674	3.5854283364
O14	2.5903052653	0.7907405722	0.7976580274
H15	0.4316780120	1.5915978641	-1.4816238738
C16	1.1619318481	2.8085269698	-2.8394022612
H17	0.2396524898	2.8865014971	-3.4057575916
H18	1.9400064527	2.1388720903	-3.1900848909
H19	1.4255003328	3.6038974132	-2.1503347273

TsD

Gasphase Energy: -1078.59501009736 hartrees

Zero Point Energy: 48.951 kcal/mol

Coordinates:

O1	1.2225804652	.9664417649	-.0931673072
V2	-.3751341328	.3867327606	-.0743091791
O3	-.7529028897	-.7229919184	-1.4553688661
O4	-1.6632882769	1.5893164783	-.1207268819
O5	-.7586719089	-.6256910310	1.3790932990
V6	-3.3830135098	.9987030169	-.1016396945
V7	-2.3543713336	-1.3759513237	1.5091570122
V8	-2.3485658263	-1.4824093339	-1.5380720130
O9	-2.5793840130	-2.3384472126	.0164652034
O10	-3.5278998917	-.0118355555	1.3509152606
O11	-2.5194467852	-2.2210513261	2.8295987177
O12	-3.5220436626	-.1107585425	-1.4810957292
O13	-4.4375312181	2.1678935038	-.1445002332
O14	-2.5079028402	-2.4180216856	-2.7967780814
C15	3.1537301107	-.6899511578	-.0806696014
H16	3.0842222945	-1.1298454647	.9122952834
H17	4.0060424137	-.0331588756	-.2453225800
H18	2.9055390150	-1.3519673704	-.9080937103
H19	2.1329956780	.2147823085	-.0860997600

ProD

Gasphase Energy: -1078.60268682583 hartrees

Zero Point Energy: 50.908 kcal/mol

Coordinates:

O1	1.4820047747	1.1239035096	-0.1175070249
V2	-0.1625238564	0.5652456428	-0.0980491167
O3	-0.5530196017	-0.5752065088	-1.4475103577
O4	-1.4827153006	1.7247273083	-0.1404337473
O5	-0.5527841218	-0.4751427172	1.3312238414
V6	-3.1992570771	1.1079773226	-0.1164849638
V7	-2.1311140277	-1.2534354698	1.4882012763
V8	-2.1319954704	-1.3639376508	-1.5458714067
O9	-2.3601980403	-2.2279772487	0.0042926984
O10	-3.3218258322	0.0987769986	1.3367639747
O11	-2.2642882247	-2.0893434408	2.8182563963
O12	-3.3220023704	-0.0041704105	-1.4929375160
O13	-4.2766669889	2.2562410737	-0.1581703771
O14	-2.2660014945	-2.2943953357	-2.8115233531
H15	2.2505817497	0.4957955180	-0.1075311109
C16	3.7335580841	-0.8291632195	-0.1005882398
H17	3.5415843748	-1.2206694657	0.8922835879
H18	4.4998794049	-0.0728108164	-0.2296575375
H19	3.4021159904	-1.3953498701	-0.9640677098

Propane

Gasphase Energy: -119.15307736604 hartrees

Zero Point Energy: 65.086 kcal/mol

Coordinates:

C1	-1.3592240615	0.1076442874	0.6051294129
C2	0.1521133872	-0.1415862911	0.5627792710
C3	0.7083879874	-0.2048333338	-0.8634928962
H4	-1.6171034119	1.0568055134	0.1209400813
H5	-1.7324382801	0.1469127902	1.6340321632
H6	-1.9060523450	-0.6862616488	0.0829342154
H7	0.3818321720	-1.0790574553	1.0858237780
H8	0.6681840924	0.6504385173	1.1209593101
H9	1.7889862845	-0.3832001477	-0.8670327304
H10	0.5240141937	0.7322809128	-1.4018374063
H11	0.2360890321	-1.0111525270	-1.4368632965

Ts-1,2

Gasphase Energy: -1157.24125223698 hartrees

Zero Point Energy: 85.401 kcal/mol

Coordinates:

O1	-0.9242460327	-0.7460160405	0.6974724123
V2	-0.8485480041	0.9319562128	0.6388402498
O3	0.8542447560	1.5642582657	0.6784154634
O4	-1.6928505738	1.8380036919	1.9030615988
O5	-1.4954096676	1.6027368606	-0.9211667429
V6	-1.6120010636	3.6478513451	1.8302575771
V7	-1.4038191047	3.3462189735	-1.1984771544
V8	1.1195899200	3.3031564651	0.5151806135
O9	0.3198972698	3.7909145487	-1.0116638877
O10	-2.2254983350	4.0951458551	0.2230165282
O11	-2.0106069719	3.7653555918	-2.5930661520
O12	0.1171934675	4.0564313512	1.8141662966
O13	-2.3973715439	4.3467634728	3.0041568378
O14	2.6485093259	3.6871936533	0.5717406727
C15	0.2770102535	-1.9863042140	-1.2083185897
C16	0.5248108036	-3.3775416638	-0.6792195640
C17	-0.6480423572	-1.8290245333	-2.3906890817
H18	1.1818977472	-1.3702907703	-1.2701887187
H19	1.1088289787	-3.3659006279	0.2452185338
H20	-0.4117184451	-3.9148033082	-0.5006343206
H21	1.0980220942	-3.9524060579	-1.4231503556
H22	-1.5875907242	-2.3708390701	-2.2434200870
H23	-0.8758025787	-0.7792030291	-2.5974705801
H24	-0.1651797963	-2.2433874384	-3.2891509038
H25	-0.3269414770	-1.3868349893	-0.2372302987

2S

Gasphase Energy: -1157.25060285070 hartrees

Zero Point Energy: 87.375 kcal/mol

Coordinates:

O1	-0.8820931076	-1.0350318895	0.8125656667
V2	-0.9083402671	0.6935729669	0.7954209652
O3	0.7495211564	1.4277310971	0.7949932341
O4	-1.7673712213	1.5956495956	2.0408472420
O5	-1.5586344270	1.3683201404	-0.7561151181
V6	-1.7600979370	3.4150617288	1.9636064170
V7	-1.5487974710	3.1083931107	-1.0633804602
V8	0.9716536346	3.1711587466	0.6290768681
O9	0.1519020769	3.6375517542	-0.8932724966
O10	-2.3992460345	3.8269552264	0.3596990452
O11	-2.1870045802	3.4779742565	-2.4577183225
O12	-0.0499362208	3.8867710123	1.9376840182
O13	-2.5646382319	4.0937455995	3.1360760091
O14	2.4897348248	3.5952561368	0.6844967968
H15	-0.4219339594	-1.5612853376	0.0861412393
C16	0.4243516029	-2.3896822006	-1.3511818280
C17	0.5318922012	-3.8032603033	-0.8751500216
C18	-0.5141369476	-2.0246328701	-2.4579685290
H19	1.3063196904	-1.7584554431	-1.2241504009
H20	1.0827159680	-3.8819886217	0.0670031464
H21	-0.4531407721	-4.2660290562	-0.7482101907
H22	1.0753292755	-4.4164612683	-1.6144980704
H23	-1.4831281900	-2.5245776361	-2.3512848586
H24	-0.6825078886	-0.9449800522	-2.5239279357
H25	-0.0991910360	-2.3405698214	-3.4304526930

2T

Gasphase Energy: -1157.25051271165 hartrees

Zero Point Energy: 87.226 kcal/mol

Coordinates:

O1	-0.6701596776	-1.0256707471	0.8458818832
V2	-0.8095176888	0.6990748695	0.8124304926
O3	0.8045821409	1.5218878425	0.7623454838
O4	-1.6851154951	1.5683094798	2.0710563325
O5	-1.5268302881	1.3261092204	-0.7226697033
V6	-1.7667775346	3.3850985057	1.9850034043
V7	-1.6110891579	3.0662692023	-1.0471556176
V8	0.9406193203	3.2721535847	0.5827199352
O9	0.0619026914	3.6832739029	-0.9256489951
O10	-2.4643464250	3.7451165605	0.3912587742
O11	-2.3071736739	3.3907154208	-2.4253344221
O12	-0.0842067343	3.9445837468	1.9111197415
O13	-2.5782587136	4.0352280778	3.1693117767
O14	2.4381647628	3.7679835768	0.6020964796
H15	-0.2553257800	-1.5654987403	0.1078633797
C16	0.4905732935	-2.4939875090	-1.3435568893
C17	0.3715311807	-3.9140025741	-0.8939712810
C18	-0.3623300206	-1.9657508807	-2.4521535174
H19	1.4498680170	-1.9998919181	-1.1773790407
H20	0.8820267665	-4.0911214982	0.0573981408
H21	-0.6751088551	-4.2233854829	-0.7971369009
H22	0.8326221602	-4.5907425901	-1.6339364695
H23	-1.3919485963	-2.3334083558	-2.3846194136
H24	-0.3827775131	-0.8714532414	-2.4807761887
H25	0.0308237294	-2.2983335137	-3.4282663361

3A (triplet)

Gasphase Energy: -1157.30530180588 hartrees

Zero Point Energy: 91.527 kcal/mol

Coordinates:

O1	-2.0347806387	-2.6906208188	0.8104002019
V2	-2.2669459292	-1.1643448147	0.4611168264
O3	-0.7513568153	-0.3335869708	0.2036162691
O4	-3.1457443865	-0.2481675714	1.7389184813
O5	-3.2538852163	-0.8977876670	-1.0225924972
V6	-3.4246490915	1.4916036342	1.4576610717
V7	-3.5433024755	0.7896517995	-1.5231804112
V8	-0.8576109969	1.4906559292	-0.2200154575
O9	-1.9433973093	1.5379462297	-1.6859732460
O10	-4.3202610032	1.5481878104	-0.0957939246
O11	-4.3963567055	0.9120854890	-2.8488618730
O12	-1.8313600812	2.2050419328	1.1481677794
O13	-4.1787426041	2.2063449605	2.6494862902
O14	1.1221263018	1.8117930742	-0.3996045816
C15	2.1855449381	0.7599328566	-0.3079493311
C16	3.2091978771	1.2076360444	0.7200937260
C17	2.7400237985	0.5095893475	-1.6993064249
H18	1.5066254950	2.6511833277	-0.6941682194
H19	1.6211550756	-0.1038256676	0.0476340361
H20	3.9557410781	0.4195112930	0.8563751835
H21	3.7374483194	2.1109396661	0.3921249827
H22	2.7379048181	1.4016959684	1.6868451614
H23	1.9474248933	0.2171027261	-2.3930445897
H24	3.2506455704	1.3963374316	-2.0934841187
H25	3.4712306125	-0.3032714076	-1.6575222859

3A (singlet)

Gasphase Energy: -1157.26576697375 hartrees

Zero Point Energy: 91.112 kcal/mol

Coordinates:

O1	-2.1773163257	-2.4253475676	0.0264576577
V2	-2.1953022180	-0.8453107918	0.0153528130
O3	-0.5522515835	-0.2212014653	-0.0413071104
O4	-3.0228449250	-0.1381741619	1.4742878460
O5	-3.1145595820	-0.1597369772	-1.3979290205
V6	-3.1429381185	1.6183966461	1.5611491180
V7	-3.2428143428	1.5955442318	-1.5037948990
V8	-0.5870389414	1.6497059540	-0.0569824516
O9	-1.4886974617	2.0741236406	-1.5008640727
O10	-3.9802214452	2.1069207728	0.0510549227
O11	-4.0224808874	2.1110985868	-2.7783504753
O12	-1.3919279070	2.0950823955	1.4361420493
O13	-3.8382920476	2.1542210782	2.8755022493
O14	1.4234586556	1.5883862042	-0.1330328354
C15	2.3478232323	0.4153509306	-0.1824830172
C16	3.2511405582	0.4636291707	1.0380826174
C17	3.0776196000	0.4324628716	-1.5148559602
H18	1.9407854554	2.4066618490	-0.1698585624
H19	1.6536679090	-0.4227879613	-0.1257103718
H20	3.8905881628	-0.4242415093	1.0541516217
H21	3.9070181490	1.3428224401	1.0191203028
H22	2.6651002423	0.4776716853	1.9606999920
H23	2.3718173822	0.4241328045	-2.3494998930
H24	3.7277975047	1.3112679904	-1.6067279400
H25	3.7109257251	-0.4563283012	-1.5956994434

3B (tiplet)

Gasphase Energy: -1157.30967037577 hartrees

Zero Point Energy: 90.667 kcal/mol

Coordinates:

O1	-0.9256688115	-2.3476879376	0.0218115837
V2	-1.1523831452	-0.5694178521	0.0100463038
O3	0.6277855707	0.4138431367	0.0194451851
O4	-1.9471173281	0.2878213456	1.4536955544
O5	-1.9208622053	0.2679928698	-1.4605677204
V6	-2.1994555065	2.0052630690	1.5140515579
V7	-2.1723897274	1.9834275181	-1.5506437127
V8	0.4543065166	2.2634692780	0.0028308232
O9	-0.4870891952	2.6843479070	-1.4143487119
O10	-2.9782189481	2.4812532185	-0.0283198451
O11	-2.9511439298	2.4030292854	-2.8598574384
O12	-0.5128322379	2.7054025529	1.3969989416
O13	-3.0003266633	2.4448559869	2.8033037843
O14	1.8758149387	2.9514978874	0.0128425688
C15	1.9331184693	-0.3079670361	0.0819797578
C16	1.9903777859	-1.0912124180	1.3849697149
C17	2.0777082044	-1.1528412995	-1.1742531564
H18	-1.6534334301	-2.9863880225	0.0113168875
H19	2.6821311632	0.4879792765	0.0887862615
H20	1.2468676969	-1.8939879979	1.3990953083
H21	2.9810638694	-1.5459627438	1.4857383224
H22	1.8295461210	-0.4332496876	2.2435879155
H23	3.0686354891	-1.6181624869	-1.1805244321
H24	1.3293616149	-1.9505280518	-1.2039753505
H25	1.9858150597	-0.5357960612	-2.0721698700

3B (singlet)

Gasphase Energy: -1157.27868827199 hartrees

Zero Point Energy: 90.274 kcal/mol

Coordinates:

O1	-1.1518556814	-2.2762891417	0.3341190164
V2	-1.0850342497	-0.5493891168	0.0020821477
O3	0.6137936576	0.3869088628	0.1606706190
O4	-1.9205163940	0.3550150908	1.2826824136
O5	-1.7749373180	0.0985188743	-1.4458928640
V6	-2.3089265083	2.0726723975	1.4212000740
V7	-2.0813133552	1.9196943893	-1.6084407285
V8	0.4478524063	2.2876792781	0.1662246954
O9	-0.4364809229	2.5796280081	-1.3487751660
O10	-3.0126320125	2.4642981122	-0.2083503017
O11	-2.7133730676	2.3336185866	-2.9949934144
O12	-0.6207984128	2.7983422926	1.4489554116
O13	-3.2132179863	2.3804532741	2.6810993939
O14	1.8573065176	3.0056653669	0.1810850213
C15	1.9295754188	-0.3070680832	0.0546887636
C16	2.1352898571	-1.1358090582	1.3128034661
C17	1.9665014370	-1.1014284011	-1.2432803505
H18	-1.8341964195	-2.8960347393	0.0371374037
H19	2.6603935299	0.5047443756	0.0140904213
H20	1.3910371716	-1.9354126989	1.3885398867
H21	3.1275087526	-1.5973395162	1.2852066944
H22	2.0752325203	-0.5082449946	2.2059361268
H23	2.9673925866	-1.5229933018	-1.3795357491
H24	1.2566951239	-1.9360642108	-1.2237965208
H25	1.7475309645	-0.4609728602	-2.1020086111

Ts-3A,4A

Gasphase Energy: -1157.25567582484 hartrees

Zero Point Energy: 86.737 kcal/mol

Coordinates:

O1	-2.6500872285	-2.4133800625	-0.3858200540
V2	-2.4942932885	-0.8383763053	-0.2995877443
O3	-0.7786825421	-0.3656054062	-0.1883605198
O4	-3.2996190285	-0.1203754368	1.1143272129
O5	-3.1618187267	0.0248255598	-1.7035194877
V6	-3.1550964210	1.6679506762	1.3368512587
V7	-3.0037632006	1.8259634836	-1.7265345955
V8	-0.4008051943	1.5057889362	-0.0744758873
O9	-1.2935077853	2.1573770790	-1.5581251079
O10	-3.7890222654	2.3441079459	-0.1982176146
O11	-3.6141634243	2.5041344107	-3.0196486768
O12	-1.4370633054	2.0042627445	1.3748356239
O13	-3.8933845537	2.2102596939	2.6277625541
O14	1.4487875650	1.3877884678	0.0326873865
H15	2.0294859613	2.1593112546	0.0977218921
C16	1.5543510546	-1.6655829084	-0.1323114297
C17	2.5154102808	-0.6952935537	0.2145187828
C18	2.9711872857	-0.4773336343	1.6060743029
H19	1.3438189698	-2.4101381275	0.6392875097
H20	1.6233899302	-2.0624213848	-1.1457863723
H21	0.4896632656	-1.0670424283	-0.1614286079
H22	3.0698981455	-0.2034329394	-0.5785104261
H23	3.7946222037	-1.1900567011	1.7769409309
H24	3.3628693386	0.5262576563	1.7705298579
H25	2.1870531095	-0.7057856071	2.3322509037

Ts-3B,4B

Gasphase Energy: -1157.25990134584 hartrees

Zero Point Energy: 86.379 kcal/mol

Coordinates:

V1	0.4804080220	-1.6703974293	1.0914454456
O2	0.5387460806	0.1010609370	1.0637571460
O3	-1.2811405902	-2.0302380124	1.0605471375
O4	1.0771920017	-2.1361110360	-0.5407017595
V5	-2.2735666474	-1.3371205480	-0.2529713844
V6	0.2677111350	-1.4576484737	-1.9795884376
V7	-0.3234338519	1.0451508202	-0.2911589929
O8	0.3649015701	0.3092817642	-1.7987796996
O9	-1.4727693604	-1.8305673865	-1.7798620640
O10	0.8727872319	-1.9858517285	-3.3431622595
O11	-2.0251461891	0.4203214333	-0.1777580692
O12	-3.7956622792	-1.7631884448	-0.1769857551
O13	0.0171240013	2.6010625639	0.1111284305
O14	1.3831674298	-2.4267214911	2.4263323183
H15	1.4012314177	-3.3900485306	2.5369236235
C16	1.3879283382	2.6845201590	2.4202517027
C17	1.6809132123	1.3397423818	2.7376253936
C18	2.9947548339	0.7091482723	2.4916398732
H19	0.6491389685	3.1658083212	3.0634826722
H20	2.2496120075	3.3062115966	2.1689247343
H21	0.9651055380	0.7813517378	3.3347617431
H22	3.6230167700	0.9754849576	3.3586745572
H23	2.9402598467	-0.3791225684	2.4522820120
H24	3.4849709075	1.1159860556	1.6033030002
H25	0.7857430304	2.6365573622	1.3747652479

Ts-3B,4C

Gasphase Energy: -1157.26058562887 hartrees

Zero Point Energy: 86.685 kcal/mol

Coordinates:

O1	0.2318620525	-1.8591870015	1.4071464013
V2	0.2850115216	0.0204281966	1.3666196002
O3	1.8646443851	0.9453794685	1.1323635952
O4	-0.7481674218	1.0962110553	2.4542591411
O5	-0.5359013527	0.2380204018	-0.3301115089
V6	-0.9514512482	2.7799622564	2.0104647850
V7	-0.7441884406	1.8831374876	-0.9085174530
V8	1.7880074175	2.6248280376	0.6303770261
O9	0.8765700455	2.6283983304	-0.9258528002
O10	-1.6520215284	2.7637398786	0.3484354927
O11	-1.4691287933	1.8449233761	-2.3265762145
O12	0.6915621960	3.4626157022	1.7762200831
O13	-1.8285509308	3.5722495293	3.0629146629
O14	3.2251740663	3.2797111865	0.5252362259
H15	0.6714511835	-2.4576696324	2.0259922407
C16	-1.0156391067	-1.7619377565	-1.6858763282
C17	-0.5480173513	-2.8657625215	-0.9505579227
C18	-2.4376183213	-1.4135222096	-1.8520717457
H19	-0.3015359033	-1.1823529141	-2.2656794896
H20	-1.3038798748	-3.6010804032	-0.6674977381
H21	0.3995975545	-3.2867337353	-1.2929009057
H22	-2.5836573352	-0.3416161374	-1.9987153651
H23	-2.7523169407	-1.9059633248	-2.7890338928
H24	-3.0637246603	-1.8058021972	-1.0472321597
H25	-0.2044575987	-2.3918794332	0.1387256110

4A

Gasphase Energy: -1039.35991273756

Zero Point Energy: 37.294 kcal/mol

Coordinates:

V1	1.6832966505	-1.4447878588	1.5584066301
O2	1.6820061384	0.5727597378	1.5518039535
O3	-0.1585866024	-1.6841619215	1.4377253408
O4	2.2457111839	-1.6814651165	-0.2004069249
V5	-1.1270962879	-1.0428441023	0.1494487024
V6	1.4020518848	-1.0414345941	-1.5739561097
V7	0.7304279609	1.4048421909	0.1583043042
O8	1.4197349183	0.7804892320	-1.3183349938
O9	-0.3243943541	-1.4850631982	-1.3903451913
O10	2.0455298382	-1.5127234050	-2.9365881354
O11	-0.8955423856	0.7787700527	0.2605543298
O12	-2.6308477254	-1.5138424304	0.2483410749
O13	0.7842303994	2.9789770693	0.2417622255
O14	2.6361973238	-2.0093881245	2.9589602389
H15	2.1310342677	1.0773271325	2.2455468935
H16	2.8038011938	-2.9296106015	3.2083456514

4B

Gasphase Energy: -1039.37227935385 hartrees

Zero Point Energy: 36.890 kcal/mol

Coordinates:

V1	1.5448274397	-1.7400221424	1.5374636786
O2	1.6183737935	0.1009829930	1.5022287864
O3	-0.1640168707	-2.1053385161	1.3968856038
O4	2.1643291205	-2.1441176253	-0.0835467135
V5	-1.1365829494	-1.3170872176	0.0627739444
V6	1.4358975741	-1.3785087267	-1.5422150453
V7	0.8490033710	1.0616687967	0.2770226012
O8	1.4929050497	0.3599178236	-1.2732139743
O9	-0.3008648333	-1.8371179663	-1.4195397932
O10	2.1212057117	-1.8102228726	-2.8972324711
O11	-0.8526421496	0.4113608873	0.2291147513
O12	-2.6709872533	-1.6841461100	0.0833812548
O13	0.9536195502	2.8138522161	0.3481232642
O14	2.4318386651	-2.3832647293	2.9083927876
H15	0.5494792758	3.3935717662	-0.3169939497
H16	3.3976736600	-2.4776518769	2.9140475981

4C

Gasphase Energy: -1039.35209737807 hartrees

Zero Point Energy: 37.577 kcal/mol

Coordinates:

O1	-0.7476467632	-2.5012594006	0.0380449698
V2	-1.0091238200	-0.9415040113	0.0253322249
O3	0.4863170999	-0.0452322714	0.0310740056
O4	-1.9672751166	-0.3509899388	1.4371421583
O5	-1.9492692686	-0.3698629451	-1.4057740388
V6	-2.3053730592	1.3932010107	1.5308688864
V7	-2.2854126323	1.3733218823	-1.5281801827
V8	0.3161436097	1.8338453192	0.0153392640
O9	-0.7048116505	2.1888287926	-1.4418810032
O10	-3.1464199124	1.7745909387	-0.0063643905
O11	-3.0912040167	1.7614590591	-2.8305373501
O12	-0.7225250676	2.2073114953	1.4548798344
O13	-3.1268408163	1.7985592234	2.8181447257
O14	2.3603368057	1.8555052262	0.0586823533
H15	2.7377565603	0.9622537007	0.1064149828
H16	3.0466957899	2.5259230017	0.1678873879

Propene

Gasphase Energy: -117.91399047257 hartrees

Zero Point Energy: 50.084 kcal/mol

Coordinates:

C1	-1.1328647322	-0.3919301477	-0.0627984025
C2	0.1951581819	-0.5119288893	-0.0601888386
C3	1.1690178551	0.6302460457	-0.0093928526
H4	-1.6175090777	0.5814703078	-0.0251596574
H5	-1.7853557065	-1.2594000622	-0.1006490446
H6	0.6330705591	-1.5103586331	-0.0995939056
H7	1.8156593699	0.5611191264	0.8749801798
H8	0.6556893964	1.5963780760	0.0195731349
H9	1.8339002627	0.6226489951	-0.8825318245

5

Gasphase Energy: -1189.68823829594 hartrees

Zero Point Energy: 42.417 kcal/mol

Coordinates:

O1	0.2087791430	-2.4924311150	1.1560943147
V2	-0.9920418761	-0.5545349556	1.3315901956
O3	0.7266867639	0.1711389392	1.5434466117
O4	-1.8032871417	0.9917457647	1.2104764743
O5	-1.0435352905	-0.9656697380	-0.4304533397
V6	-1.3781263323	2.3595689626	0.0975168639
V7	-0.4240720030	0.1192231265	-1.6989682950
V8	1.4210920213	1.2887846018	0.4180186693
O9	1.2199862240	0.5857500046	-1.2407662388
O10	-1.4214251280	1.6062866481	-1.5121075365
O11	-0.5183856397	-0.4971292822	-3.1471049713
O12	0.3101168322	2.7259661243	0.4493429888
O13	-2.3179647561	3.6179624115	0.2168907439
O14	2.9174531856	1.6289400098	0.7815722005
O15	-2.0527351594	-1.4791713621	2.4008456763
O16	-0.8755180844	-1.1261194517	3.0865383215
H17	0.3101050220	-2.8822029963	2.0370652004
H18	-0.2083260512	-3.1496456097	0.5818238842

6 (singlet)

Gasphase Energy: -1113.24945003507 hartrees

Zero Point Energy: 26.674 kcal/mol

Coordinates:

V1	-0.3217075446	-0.7691015424	0.7665146175
O2	-0.3188117173	0.9583952062	0.5102519714
O3	-1.9564672478	-1.3498352701	0.5671557070
O4	0.2863586368	-1.2433984411	-0.9671135909
V5	-3.0229530871	-0.7631843648	-0.7908337940
V6	-0.4826310225	-0.7340331290	-2.4221619226
V7	-1.2562400470	1.7261553372	-0.8524051614
O8	-0.5432828006	1.0868277401	-2.3237530361
O9	-2.2189996869	-1.2723899142	-2.2660236061
O10	0.2579522731	-1.2918121405	-3.6953405032
O11	-2.8983898253	1.0214646619	-0.7586565052
O12	-4.5078846412	-1.2734116224	-0.7038387040
O13	-1.2630632892	3.2982644308	-0.8165377521
O14	0.2967410020	-1.1687748954	2.3713626023
O15	1.0820465030	-1.7517847278	1.3565808541

6 (triplet)

Gasphase Energy: -1113.24433429820 hartrees

Zero Point Energy: 24.891 kcal/mol

Coordinates:

V1	-0.2383226404	-0.7280982077	0.6738815035
O2	-0.3413238904	0.9859934212	0.5251487013
O3	-1.9859878438	-1.2692460910	0.5755985499
O4	0.3305839175	-1.2672913006	-0.9850156959
V5	-3.0189809100	-0.7560545297	-0.7477002683
V6	-0.5025126681	-0.7530437991	-2.4394990265
V7	-1.2853598820	1.7424283177	-0.8821812959
O8	-0.5624323600	1.0659357036	-2.3371649571
O9	-2.2074545329	-1.2647597386	-2.2574241058
O10	0.1805430310	-1.3081051756	-3.7459064721
O11	-2.9045169384	1.0625179127	-0.7603212303
O12	-4.4862457376	-1.3124023542	-0.6107127896
O13	-1.2840589796	3.3162858745	-0.8769551772
O14	0.1359901059	-1.5612714570	2.4010841323
O15	1.2189394613	-1.5786968279	1.6534693049

6 (quintet)

Gasphase Energy: -1113.20151698957 hartrees

Zero Point Energy: 25.216 kcal/mol

Coordinates:

V1	-0.7409186425	-1.0378470892	0.6808629074
O2	-0.5737698893	0.7768358754	0.7603319568
O3	-2.4850208303	-1.3412863178	0.3195007544
O4	0.1524374368	-1.5313824946	-0.8246598229
V5	-3.2035162244	-0.5779203901	-1.1121059133
V6	-0.4113796767	-0.7720735392	-2.3378546870
V7	-1.1820478087	1.6680119513	-0.6549298514
O8	-0.2805608467	0.9885966320	-2.0470543259
O9	-2.1683781120	-1.0876588444	-2.4845655185
O10	0.4152964845	-1.2571793900	-3.5910739346
O11	-2.8843547318	1.1748941033	-0.9244399997
O12	-4.7302473777	-0.9284718120	-1.3026789192
O13	-1.0026183750	3.2276900426	-0.4974234299
O14	2.1662343826	-0.9775582070	2.1044371743
O15	1.0542287508	-1.4586985584	2.1602897478

Ts-6,7

Gasphase Energy: -1232.37634362330 hartrees

Zero Point Energy: 87.562 kcal/mol

Coordinates:

V1	0.2424725687	-1.4988559883	0.0639895908
O2	0.4714028865	0.3169047978	0.1531729887
O3	-1.4825550103	-1.7553233236	-0.1120155116
O4	0.8065409296	-1.7624671499	-1.6813617156
V5	-2.4171046993	-0.8168172596	-1.3681478760
V6	0.1202777684	-0.9072029963	-3.0294559464
V7	-0.2891652611	1.3562289588	-1.0530988118
O8	0.3145392927	0.8411029624	-2.6465803543
O9	-1.6733623695	-1.1991465871	-2.9209598428
O10	0.7691639892	-1.3297759950	-4.4044916635
O11	-2.0362572019	0.8861687917	-1.0491694141
O12	-3.9663022006	-1.1061251866	-1.3422696498
O13	-0.0370411544	2.8862862305	-0.7555051907
O14	0.8972623074	-1.9043417934	1.8955071535
O15	1.4395676204	-2.6604714459	0.8060462976
H16	1.7590791148	-1.1106603395	2.2503730682
C17	2.6955012823	-0.2221890069	2.6446627330
C18	3.7877617203	-1.0906449681	3.2102754670
C19	1.9514415661	0.7072670766	3.5664519776
H20	2.9091354717	0.2000466581	1.6570834646
H21	4.6518863277	-0.4596411882	3.4716572716
H22	3.4704377832	-1.6031087783	4.1237417482
H23	4.1372473548	-1.8330930018	2.4870472928
H24	1.1061491546	1.1844875812	3.0637070232
H25	1.5963636412	0.1946889048	4.4666155616
H26	2.6306952833	1.5088230205	3.8967351298

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Gasphase Energy: -1232.38001280938 hartrees

Zero Point Energy: 89.952 kcal/mol

Coordinates:

V1	0.0615644560	-1.7139868504	0.1061218137
O2	0.0334589494	0.1175737741	0.2013868406
O3	-1.6185549445	-2.2136631715	0.0637497865
O4	0.5162105476	-1.8936468489	-1.6636883608
V5	-2.7732236035	-1.4108958338	-1.1019046261
V6	-0.3845649648	-1.1349411651	-2.9538336151
V7	-0.9553922344	1.0425914502	-0.9248353079
O8	-0.4108103533	0.6184114392	-2.5709603370
O9	-2.1002888461	-1.6839768788	-2.7112803713
O10	0.2058830246	-1.4563461787	-4.3803451732
O11	-2.6124407956	0.3276857123	-0.7932060881
O12	-4.2594622533	-1.9157939818	-0.9628847885
O13	-0.8976599186	2.5915148467	-0.6254623997
O14	0.8356763196	-1.9718302317	1.9855837178
O15	1.4278388713	-2.6549309437	0.8418313529
H16	1.5047012794	-1.2288753157	2.2173289417
C17	2.5981154462	0.1231934977	2.6311179532
C18	3.6955838380	-0.5756793713	3.3704047907
C19	1.6576992626	1.0429783657	3.3453361883
H20	2.7716582070	0.3341442721	1.5735043607
H21	4.4982996367	0.1386132209	3.6216554330
H22	3.3447795652	-0.9994101014	4.3183876347
H23	4.1550961513	-1.3706152906	2.7749926260
H24	2.1699817140	1.9884142312	3.5952114746
H25	0.7947272010	1.3039549609	2.7252258707
H26	1.3077429058	0.6174261915	4.2931205497

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Gasphase Energy: -1232.50466714025 hartrees

Zero Point Energy: 92.819 kcal/mol

Coordinates:

V1	0.1980747170	-0.3378401408	1.2626587627
O2	0.2300469147	1.3780339699	0.9794257863
O3	-1.3952815668	-0.9642439802	0.9780180030
O4	0.2681788111	-0.4038123661	-1.0820349480
V5	-2.7756007303	-0.1317309420	0.0923128711
V6	-0.7733703458	0.3295774274	-2.1262753840
V7	-1.0255849608	2.3736125882	0.0892190104
O8	-0.7541395922	2.1197259512	-1.5970418724
O9	-2.4466841696	-0.3074006574	-1.5924217348
O10	-0.3748028741	0.0455607807	-3.6363845066
O11	-2.5981271367	1.6054548843	0.4857090097
O12	-4.1991965526	-0.7012902566	0.4638040133
O13	-0.9881457857	3.9076742669	0.4542046227
O14	0.2291989276	-0.3759531602	3.0182305641
O15	1.6010377845	-1.2562012824	0.9802278229
C16	2.4080714544	-2.0032378560	0.0263763530
C17	1.7441449776	-3.3488435841	-0.2263812760
C18	3.8122391831	-2.0890072344	0.6124843108
H19	-0.4818947773	0.0499599747	3.5246473370
H20	2.3958712721	-1.3955128453	-0.8830144389
H21	1.6821749810	-3.9332824167	0.6967670636
H22	0.7406448909	-3.2094898607	-0.6350268141
H23	2.3360644497	-3.9121029850	-0.9547214654
H24	3.8129895908	-2.6622325903	1.5440345151
H25	4.4671819776	-2.5911862620	-0.1064777039
H26	4.2151199873	-1.0923201546	0.8089133759

Ts-8,1

Gasphase Energy: -1232.45693062019 hartrees

Zero Point Energy: 89.923 kcal/mol

Coordinates:

O1	-2.8125207004	-1.0826250955	0.6953010764
V2	-4.3502211014	-0.8331173397	0.4182398763
O3	-4.7438638055	0.8393133905	0.2927398294
O4	-5.4380256444	-1.4016657032	1.7285190840
O5	-4.9563638502	-1.5044198509	-1.1643205631
V6	-7.1095000416	-0.8117455609	1.5245518357
V7	-6.5825731815	-0.9651519100	-1.5802049180
O8	-6.4400582341	0.8321009340	-1.6937489062
O9	-7.5844054759	-1.3124415845	-0.1529941081
O10	-7.1287141908	-1.6326384041	-2.9035845206
O11	-6.9961685778	0.9258031175	1.4983356373
O12	-8.0946956696	-1.3194803542	2.6539820169
V13	-6.4021547640	1.6844755205	-0.1377087790
O14	-8.2174663451	2.2038133406	-0.2354236167
O15	-5.8305988822	3.1935966982	-0.2417243601
C16	-6.7830263470	5.1261500632	-0.4836824099
C17	-8.1711323600	4.8730708352	-0.3578364663
C18	-6.1202670055	5.4165891018	-1.7767381943
H19	-8.7538391681	1.9081126680	0.5166657793
H20	-8.2388181931	3.6598315143	-0.2957734568
H21	-6.2116854971	5.3341505419	0.4169236302
H22	-8.7683740217	5.0971767626	-1.2442118331
H23	-8.6198151727	5.1945851880	0.5837184682
H24	-6.1773441811	6.5083143566	-1.9150538586
H25	-5.0665744613	5.1353005065	-1.7671276664
H26	-6.6355340680	4.9461243010	-2.6175239866

O_2 (tiplet)

Gasphase Energy: -150.31662157822 hartrees

Zero Point Energy: 2.375 kcal/mol

Coordinates:

O1	0.6071179418	0.0000000000	0.0000000000
O2	-0.6071179418	0.0000000000	0.0000000000

H_2O

Gasphase Energy: -76.41813386966 hartrees

Zero Point Energy: 13.413 kcal/mol

Coordinates:

O1	-0.3314525538	0.0000000000	0.4699450580
H2	0.6323633904	0.0000000000	0.4232602720
H3	-0.6093103077	0.0000000000	-0.4541297546

Part 2. Frequency calculation results for the singlet, triplet, and quintet 6

6 (singlet)

128.92
146.1
152.26
169.37
176.34
191.78
194.91
197.06
201.41
206.01
208.02
216.51
224.65
242.1
276.88
282.99
285.09
287.88
290.2
303.56
306.71
459.59
522.08
538.87
568.65
626.55
645.12
671.25

676.07

690.02

714.67

737.67

890.68

892.24

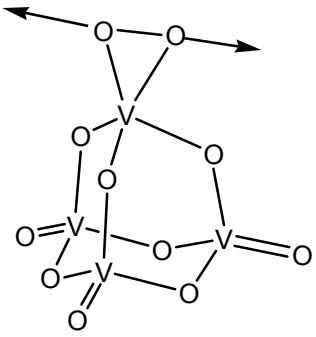
906.25

1042.02 (O-O stretch on O-V-O three membered ring)

1121.83

1124.89

1141.85



singlet state
ν(O-O stretch) = 1042 cm^{-1}

6 (triplet)

106.61

112.2

114.8

157.08

170.12

187.41

191.57

192.98

196.64

199.17

206.82

208.83

216.0

218.97

262.06

275.27

282.45

288.58

297.26

298.67

303.81

444.51

501.99

523.78

546.72

556.32

612.9

632.6

682.95

686.23

696.46

699.87

846.42

872.02

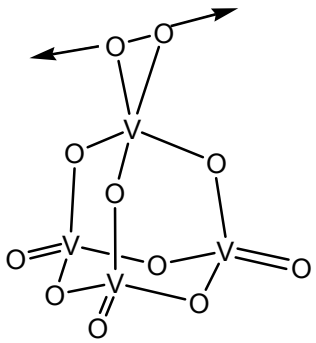
890.83

1120.43

1121.64

1138.78

1233.34 (O-O stretch on O-V-O three membered ring)



triplet state

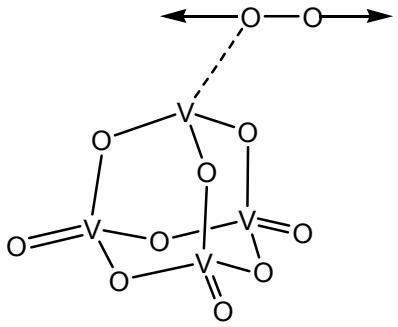
ν(O-O stretch) = 1233 cm^{-1}

6 (quintet)

12.65

34.12

77.43
101.49
159.52
164.52
175.65
191.16
194.29
196.97
199.6
204.06
207.19
216.32
219.46
229.38
260.64
269.9
292.71
293.41
310.47
315.31
316.07
484.83
536.87
567.87
585.62
640.78
659.67
665.15
694.88
702.96
751.1
847.67
849.78
1115.34
1115.61
1133.81
1644.94 (O-O stretch on O_2 fragment)



quintet state

ν(O-O stretch) = 1644 cm^{-1}